Effect of Structural Heat Conduction on the Propagation of Flames in Microchannels

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Work Supported by the Air Force Office of Scientific Research
AFOSR F496200110435
Dr. Mitat Birkan

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **21 JUN 2004**	2. REPORT TYPE **N/A**	3. DATES COVERED **-**
4. TITLE AND SUBTITLE **Effect of Structural Heat Conduction on the Propagation of Flames in Microchannels**		5a. CONTRACT NUMBER 5b. GRANT NUMBER 5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)		5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **University of Maryland College Park**		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR’S ACRONYM(S) 11. SPONSOR/MONITOR’S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES
See also ADM001793, International Symposium on Energy Conversion Fundamentals Held in Istanbul, Turkey on 21-25 June 2005., The original document contains color images.

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**UU**	**43**	

Motivation

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- Propulsion systems for Nano and Pico-satellites
  - 0.1 to 10 kg
  - High energy density of chemical propellants is attractive
  - Combustion well established means for energy release
- Behavior of deflagration wave may be different when stabilized in small passages
  - Increased exchange with structure
    - *Quenching*
    - *Increased burning rate*
    - *Enhanced flame stability*
  - Potentially important effects on performance of micro-rocket motors

Previous Work: Fundamental

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- Quenching in small passages
  - Zeldovich (1941)
  - Lewis and Von Elbe (1961)
- Effect of heat loss on RR and flammability limits
  - Spalding (1954)
    - *Heat loss decreases burning rate and broadens flammability limits*
- Effect of heat recirculation (excess enthalpy burners)
  - Weinberg (1970)
  - Weinberg and Hardesty (1974)
  - Takeno(1979,81)
    - *Constant T walls, single-step reaction*
  - General observations:
    - *Super-adiabatic flame temperatures*
    - *Elevated burning rates*

Previous Work: Micro-Channels

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- Burning rate and flammability measurements in conductive tubes
  - Zamaschikov (1997)
    - *Combustion below 'quenching limit' possible*
- Model of flame propagation in a narrow, conductive, channel
  - Zamaschikov and Minaev (2001)
    - Fast chemistry
    - Conduction broadens flammability limits
    - Hysteresis possible
- Minimum 'practical' volume for an HCCI combustor
  - Aichlmayr (2002)
    - *Thermal coupling between gas and structure*
    - *Full chemistry*
    - *No conduction within structure*
- Effect of velocity, heat loss, and passage width on burning rate in microchannel
  - Matalon and Daou (2002)
    - *Constant T walls, single-step overall reaction*
    - *Heat loss to environment decreases burning rate*
- Effect of axial conduction in heat recirculating burner
  - Ronney (2003)
    - *PSR with full chemistry*
- Effect of axial conduction in silicon micro-combustor
  - Current work: Effect of heat transfer within structure (conduction)

Objective

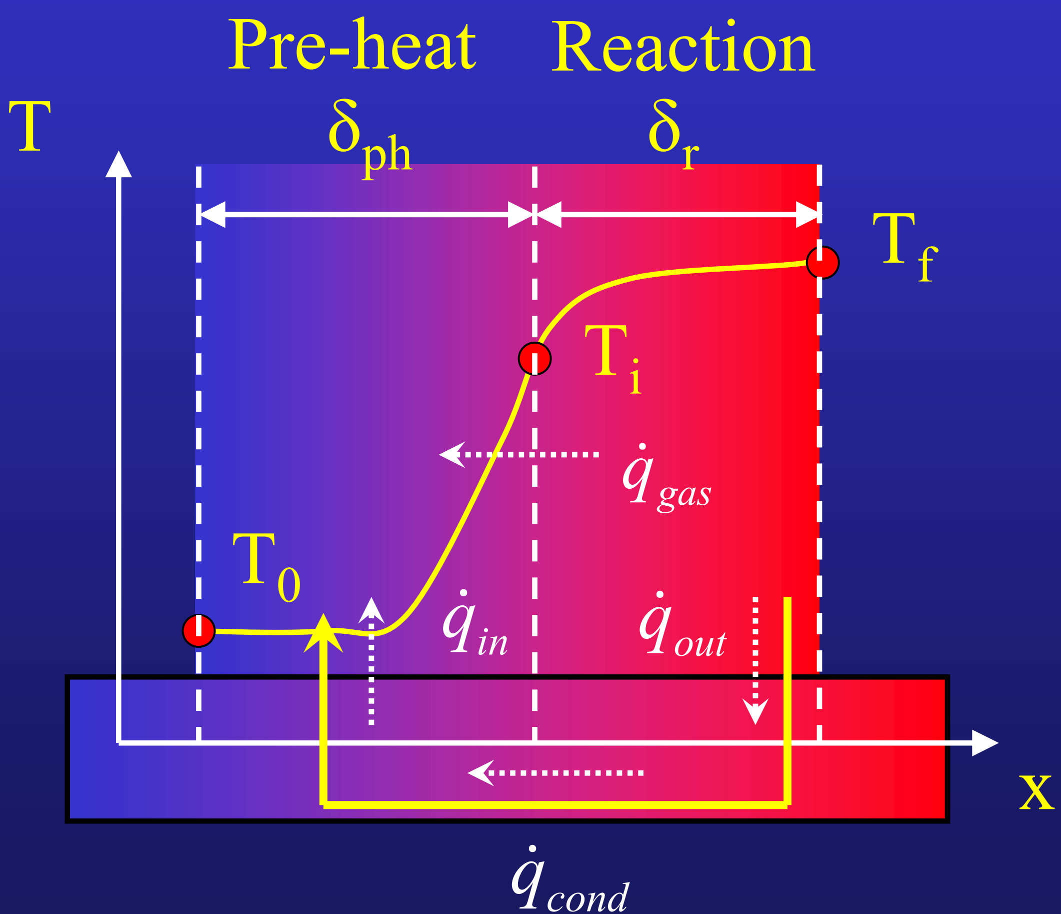
- Investigate physics of fluid structure coupling that occurs in chemically reacting systems operating at micro-scales.
  - Enable development of small, efficient combustors for micro rocket motors
  - How small can *practical* micro-rockets be built?
    - *Efficient and stable combustion*
  - What level of performance is available?
    - *Thrust/weight (power density)*
    - *Specific impulse (efficiency)*

Approach

- Modeling and Simulation
  - Simple model for effect of thermal coupling on δ_r
    - *Modification of Mallard-Le Chatelier approach*
  - Numerical simulation
    - *1-D geometry, Full chemistry, Conjugate heat transfer, Heat conduction in structure*
- Experiments
  - Develop novel non-intrusive diagnostic technique
  - Investigate behavior in parallel plate flow reactor with conductive, temperature-controlled walls

Analytical model

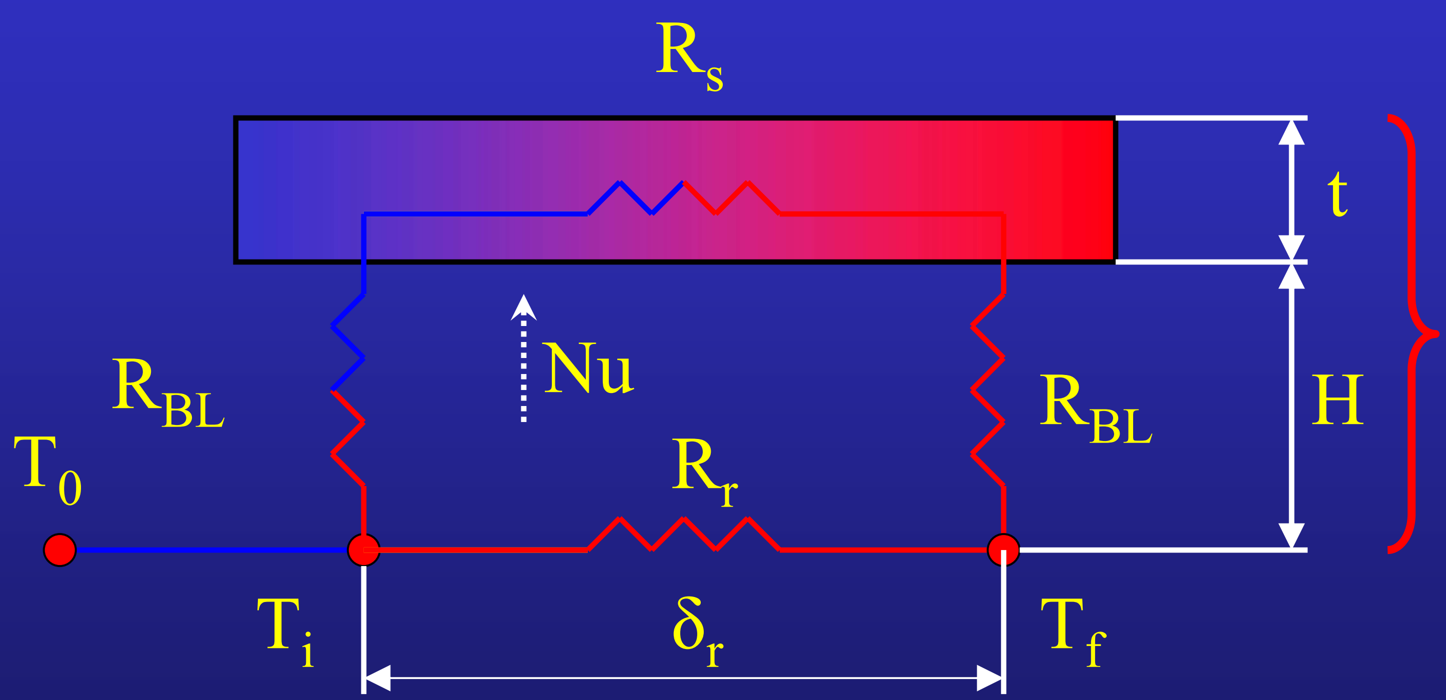
- Include thermal coupling with structure:



Structure provides another path for heat transfer

Analytical model

- Thermo-electrical analogy:



Conduction area ratio:

$$\zeta \equiv \frac{A_s}{A_r} = \frac{2t}{H}$$

(Parallel plate)

$$R_r = \frac{\delta_r}{k_r A_r} \qquad R_s = \frac{\delta_r}{k_s A_s} \qquad R_{BL} = \frac{1}{h_T A_{CONV}}$$

Analytical model

- Flame thickness:

$$\delta_r = \sqrt{\beta}\underbrace{\sqrt{\frac{k_r}{\rho C_p}\frac{T_f - T_i}{T_i - T_0}\frac{1}{RR}}}_{\delta_{r,fr}} \quad \text{with} \quad \beta = \frac{1+\zeta\frac{k_s}{k_r}\left(1+\frac{4H}{\delta_r}\frac{1}{Nu}\right)}{1+4\zeta\frac{k_s}{k_r}\frac{H}{\delta_r}\frac{1}{Nu}}$$

- Asymptotic behavior:
  - Nu → 0 or H → ∞: No thermal coupling

$$\delta_r \rightarrow \delta_{r,fr}$$

  - Nu → ∞ or H → 0: Perfect thermal coupling

$$\frac{\delta_r}{\delta_{r,fr}} \rightarrow \sqrt{1+\frac{k_s}{k_r}\zeta} > 1$$

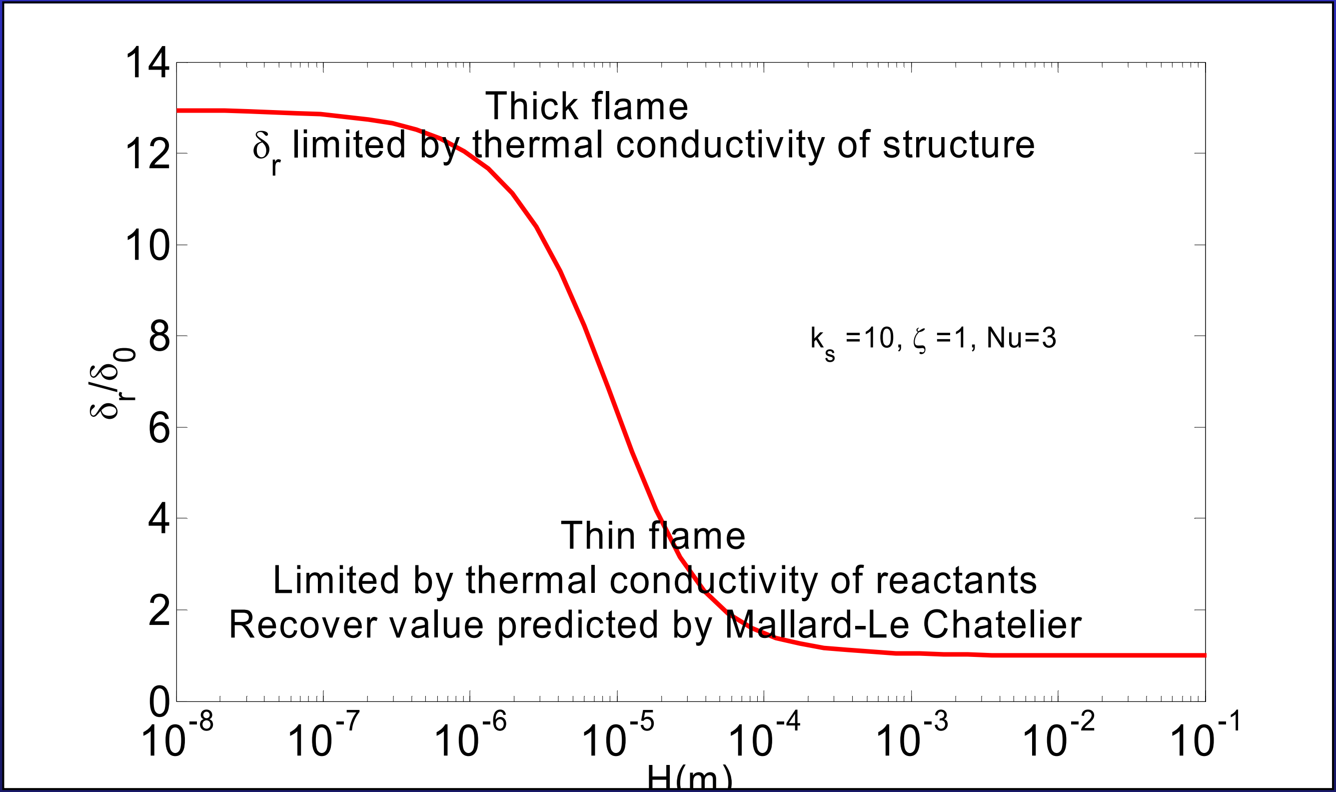
Limit-cycle behavior of δ_r in H

Large H: limited by k_r (thin flame)

Small H: limited by k_s (thick flame)

Analytical model

- Solving for δ_r ⇔ third order polynomial

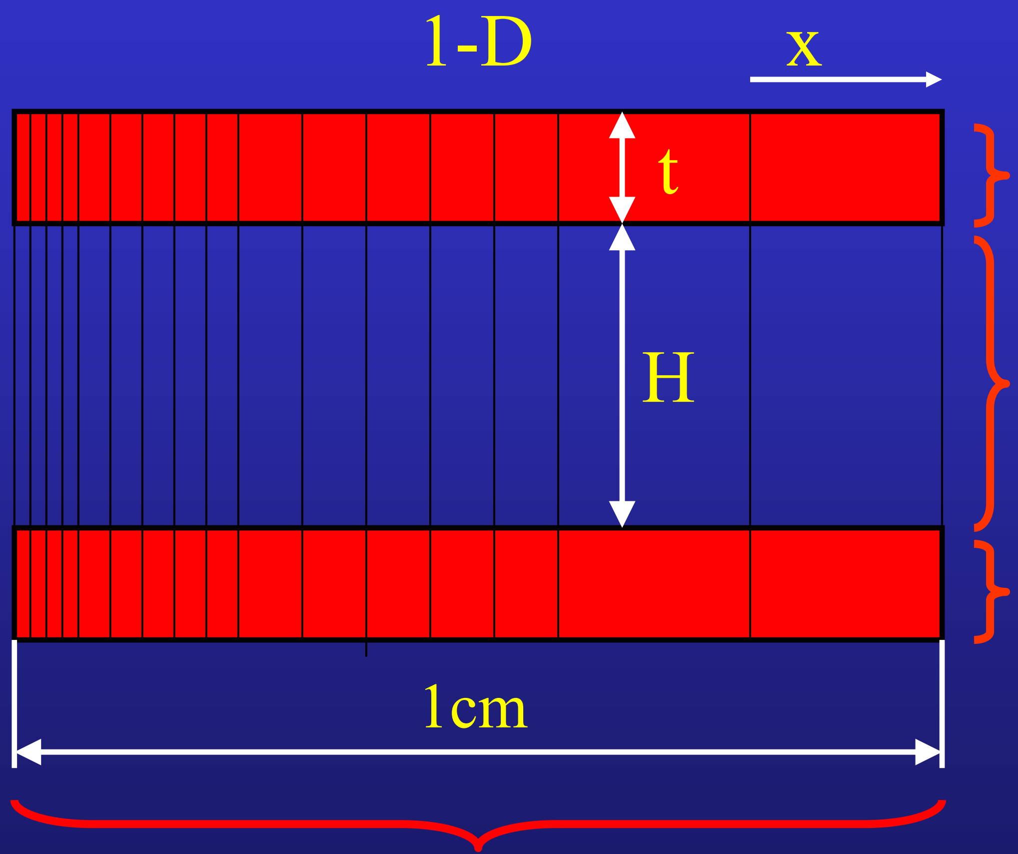


Questions:

- Influence of Nu?
- Influence of k_s?

Numerical Simulation

T_0=300K
P=1atm
H_2-air
Φ=0.5



Structure: Energy

Gas-phase:
- Continuity
- Energy
- Species

Structure: Energy

201 grid points
Unevenly spaced mesh

Numerical Simulation

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- Differences wrt. analytical model:
  - Chemistry (9 species and 19 reactions)
  - Include species diffusion
  - Transient capability, but consider steady-state solution
- Assumptions:
  - 1-D
  - P=const
  - Laminar, incompressible, inviscid
  - Nu=const
  - No thermal diffusion
  - Fourier conduction and Fickian diffusion
  - $\zeta \equiv A_s/A_r = 1$
  - Adiabatic and non-adiabatic operation

Numerical Simulation

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State

$$\rho = \frac{PW_m}{RT}$$

Mass

$$\frac{d(\rho u)}{dx} = \rho \sum_k \left(\frac{W_m}{W_k} \frac{dY_k}{dt} \right) + \frac{\rho}{T} \frac{dT}{dt}$$

Energy (gas)

$$\rho C_P \frac{dT}{dt} = -\rho u \frac{d\left(\sum_k (h_k Y_k) \right)}{dx} + \frac{d}{dx}\left(k_r \left(\frac{dT}{dx} \right) \right) - a_{ch} h_T (T - T_s) - \sum_k (W_k h_k \dot{\omega}_k)$$

Species (gas)

$$\rho \frac{dY_k}{dt} = \frac{d}{dx}\left(\rho D_k \frac{dY_k}{dx} \right) - \rho u \frac{dY_k}{dx} + W_k \dot{\omega}_k$$

Energy (structure)

$$\rho_s C_{P,s} \frac{dT_s}{dt} = \frac{d}{dx}\left(k_s \left(\frac{dT_s}{dx} \right) \right) + a_s h_T (T - T_s) - a_s h_{T,e} (T_s - T_e)$$

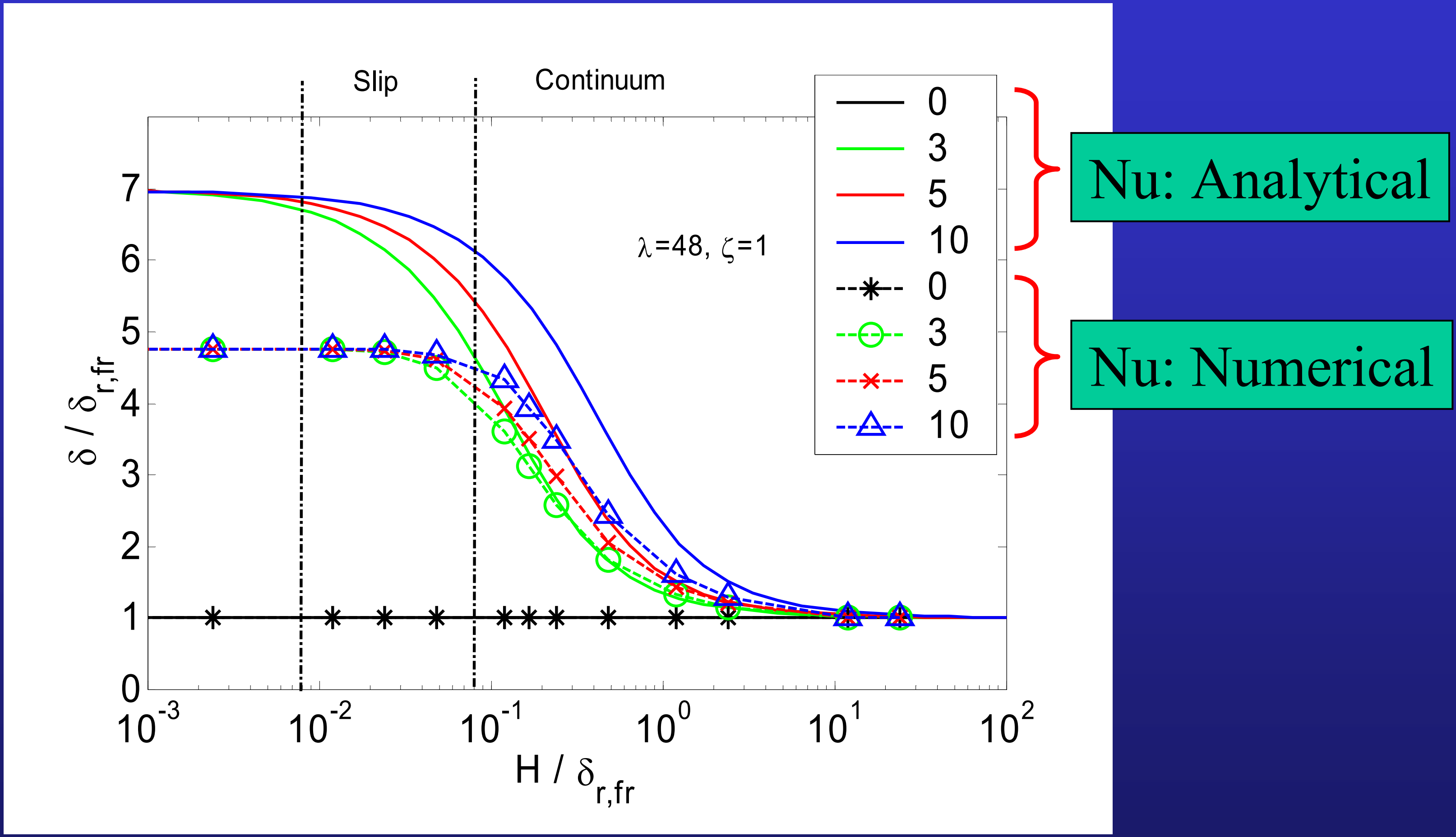
Flame Thickness

- Estimate based on temperature change through the flame*

$$\boxed{\delta_r = \frac{T_f - T_0}{\left(\dfrac{dT}{dx}\right)_{\max}}}$$

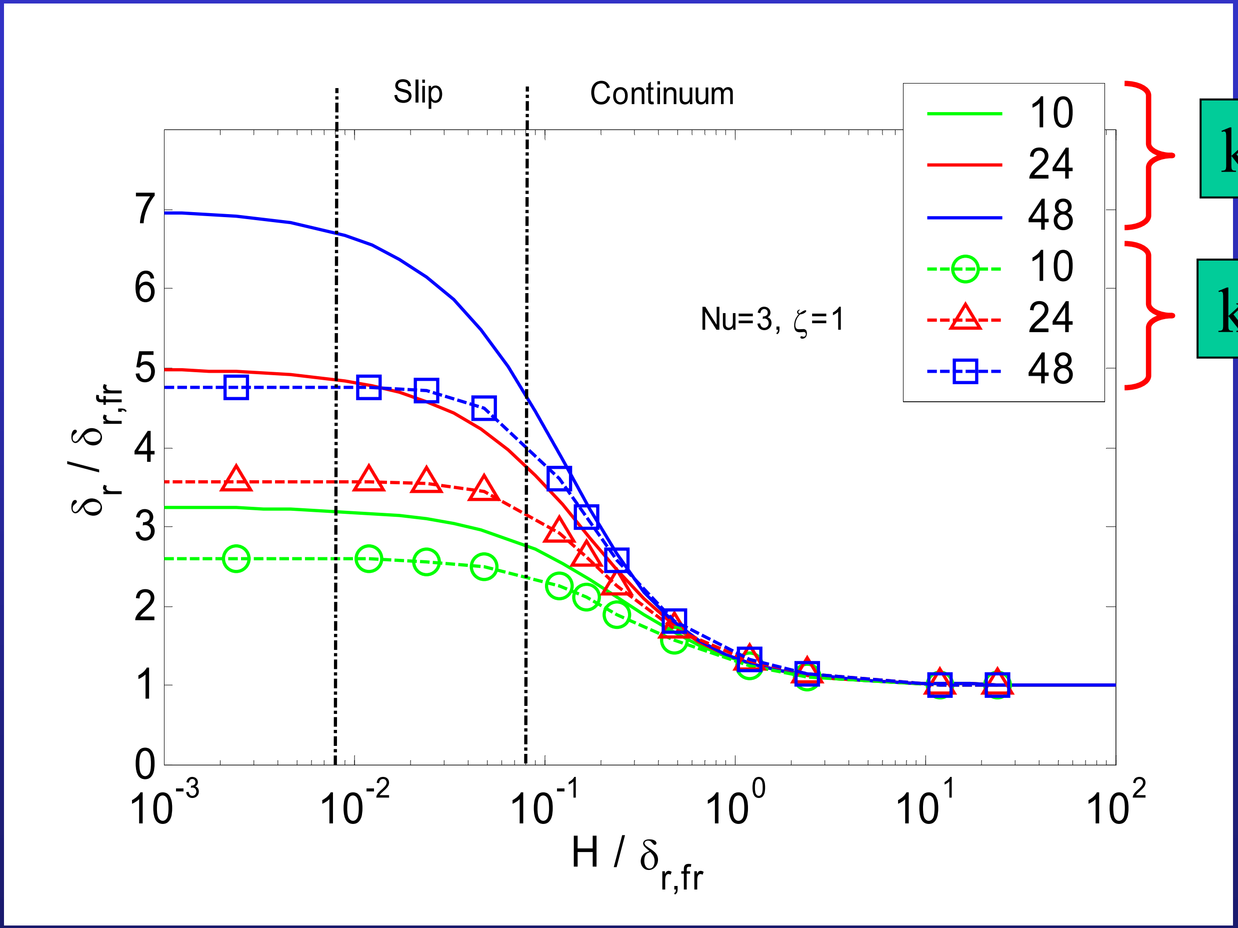
* Law, C.K. and Sung, C.J., 'Structure, Aerodynamics, and Geometry of Premixed Flamelets', Progress in Energy and Combustion Science 26 (2000) 459-505

Effect of Nusselt Number



- *Increasing Nu causes broadening to occur at larger H*
- *Consistent with model predictions*

Effect of Thermal Conductivity

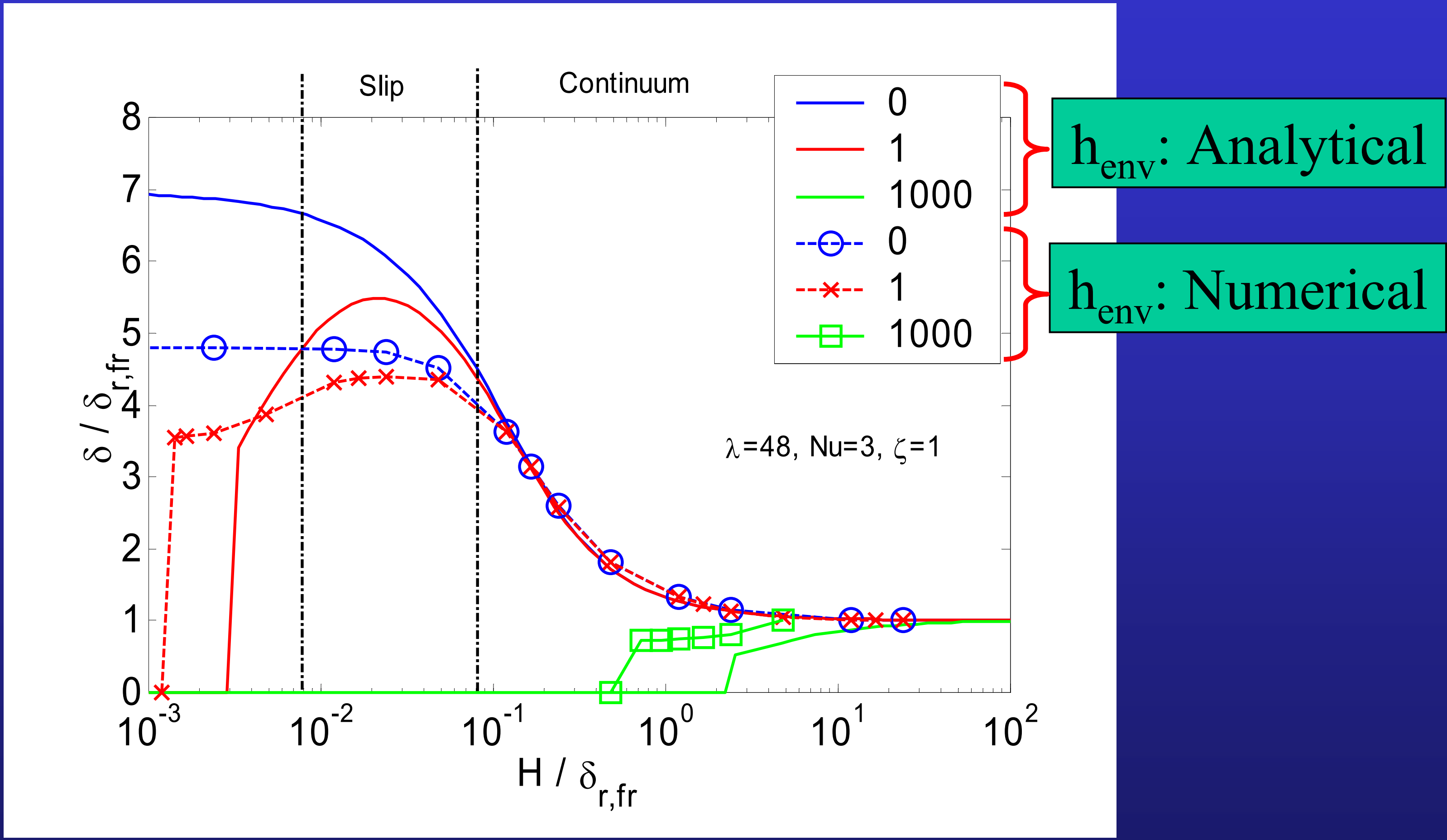


k_s: Analytical

k_s: Numerical

- *Increasing k_s increases broadening effect*
- *Consistent with model predictions*

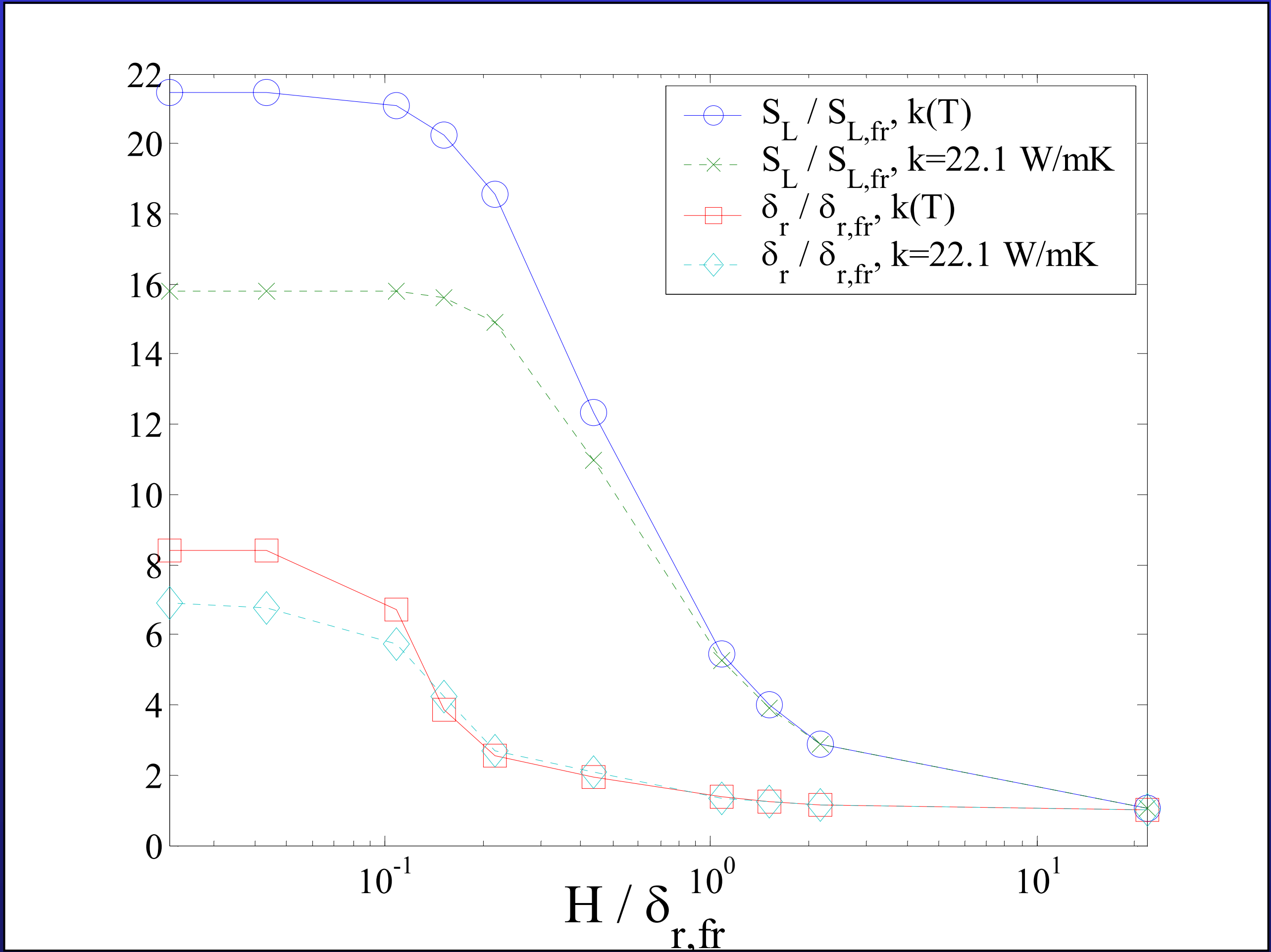
Effect of Heat Loss



- *Heat loss reduces broadening and leads to quenching*
- *Consistent with model predictions*

Silicon Micro-Combustor

U N I V E R S I T Y O F M A R Y L A N D



- *Conduction also increases burning rate.*
- *Including $k_{si}(T)$ is important*

Silicon Micro-Combustor

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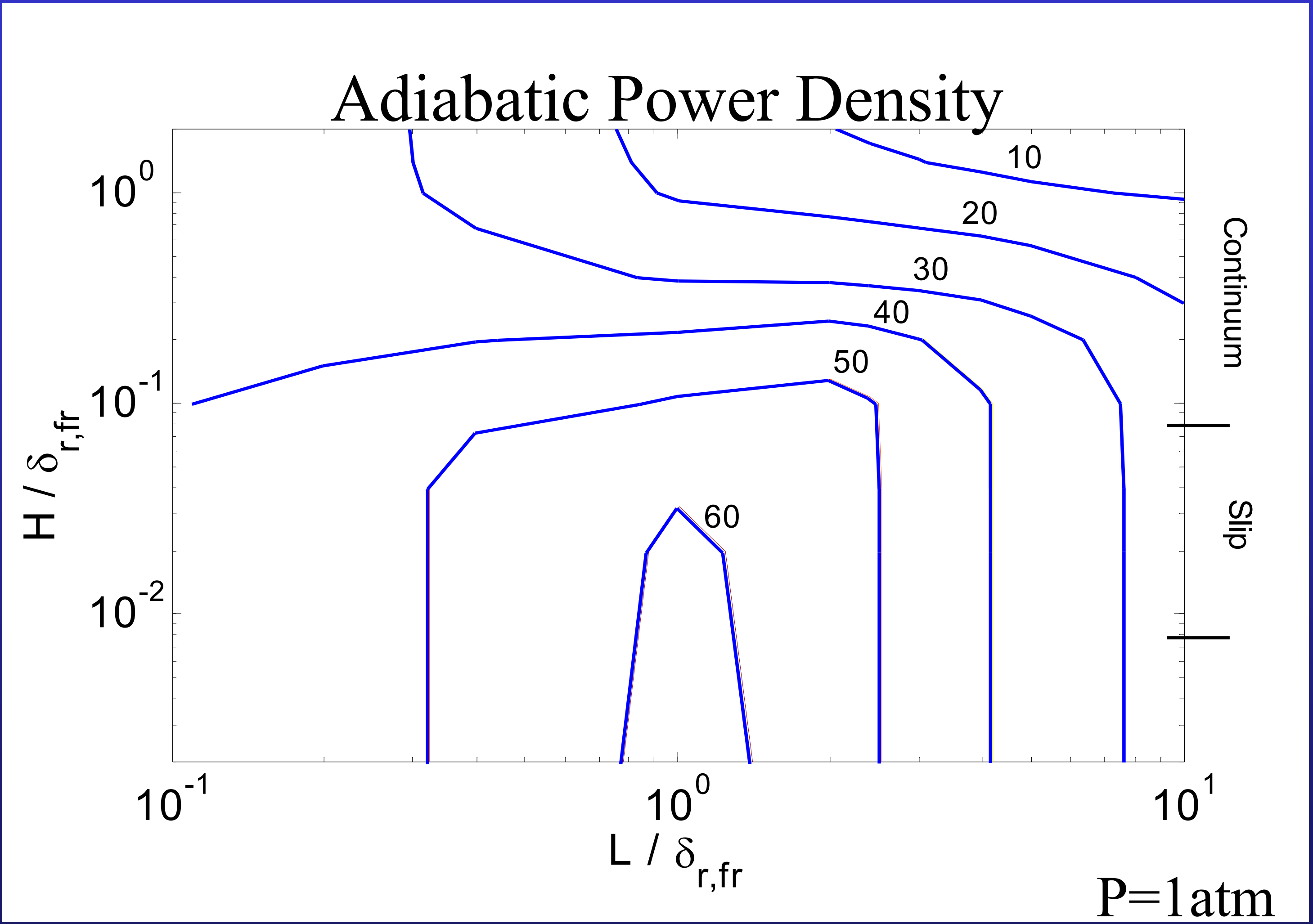
Definition of Power Density

$$\dot{w}_D = \frac{\rho S_L \int_{T_o}^{T_f} C_p(T)\,dT}{L}$$

Note: In following plots, power density is non-dimensionalized by a 'reference' value corresponding to combustion at the laminar flame speed S_L in a volume of 1 cm^3.

Silicon Micro-Combustor



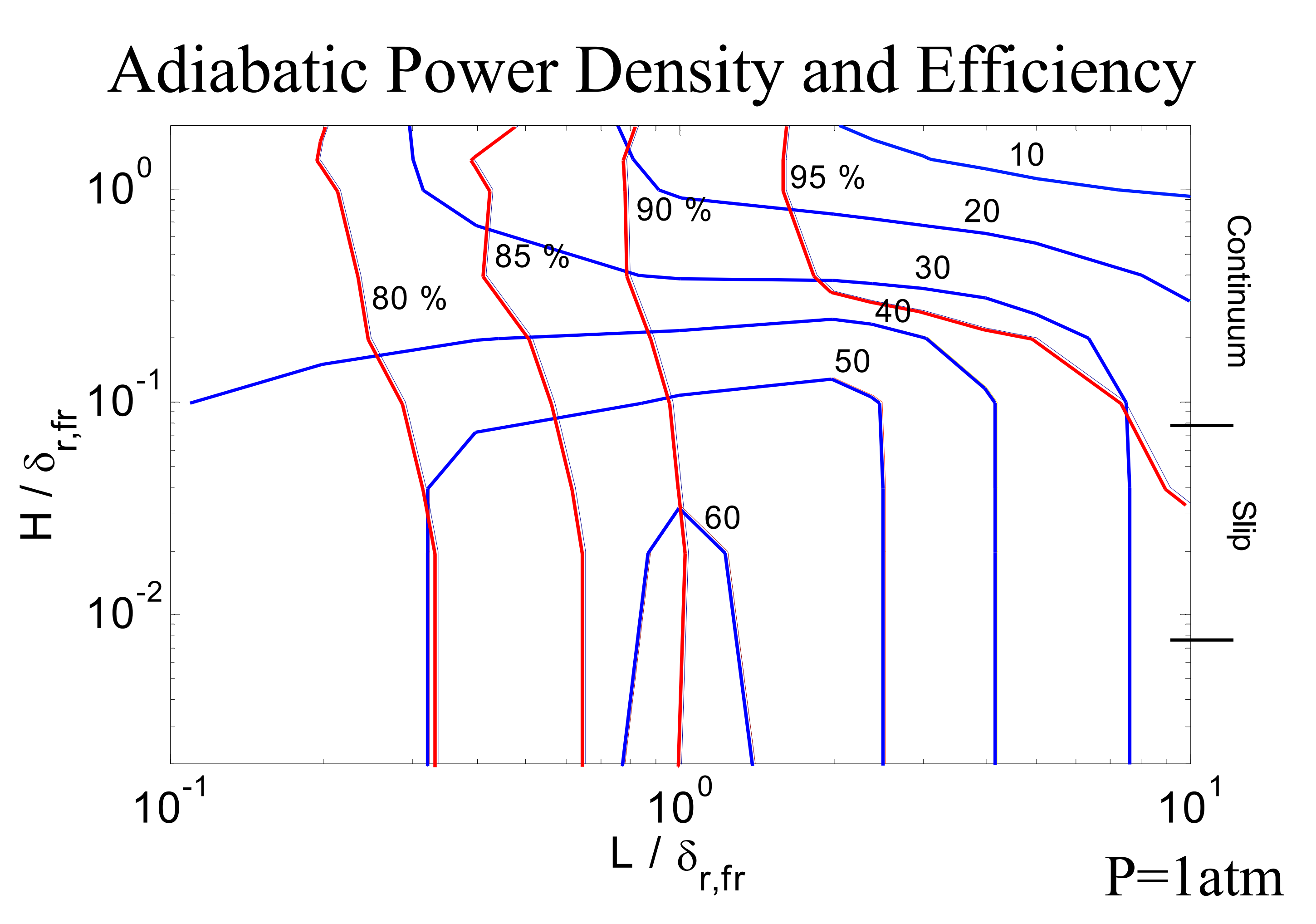
Power density increases as reduce H; optimum L

Silicon Micro-Combustor

Definition of Efficiency

$$\eta = \frac{\dot{m}_{f+a} C_P \left(T_{out} - T_{in} \right)}{\dot{m}_f Q_R}$$

Silicon Micro-Combustor



Config. That maximizes power density does **not** *maximize efficiency.*

Silicon Micro-Combustor

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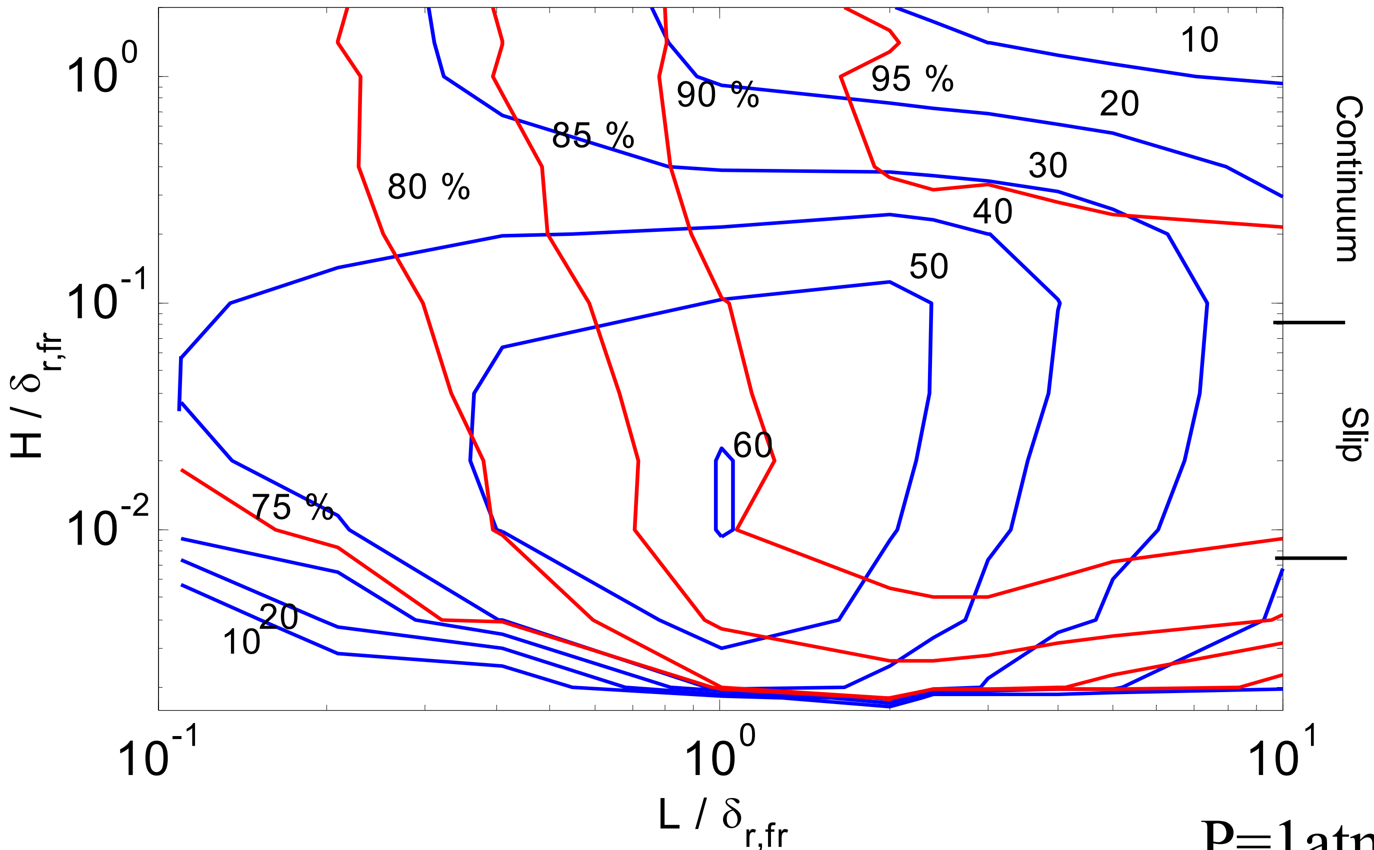
Non-adiabatic Power Density and Efficiency



P=1atm

Including heat losses leads to optimum H and L

Silicon Micro-Combustor

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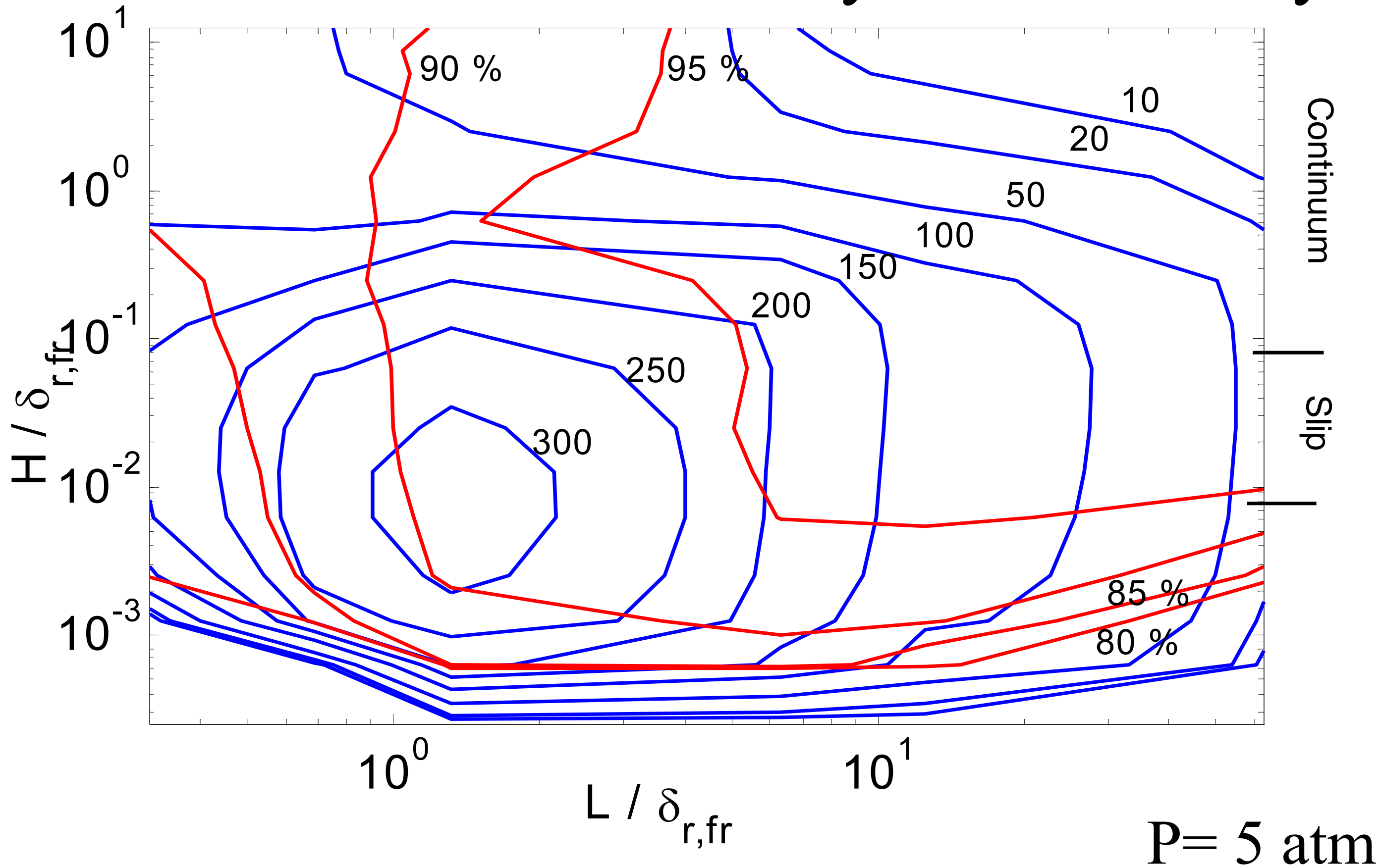
Non-adiabatic Power Density and Efficiency



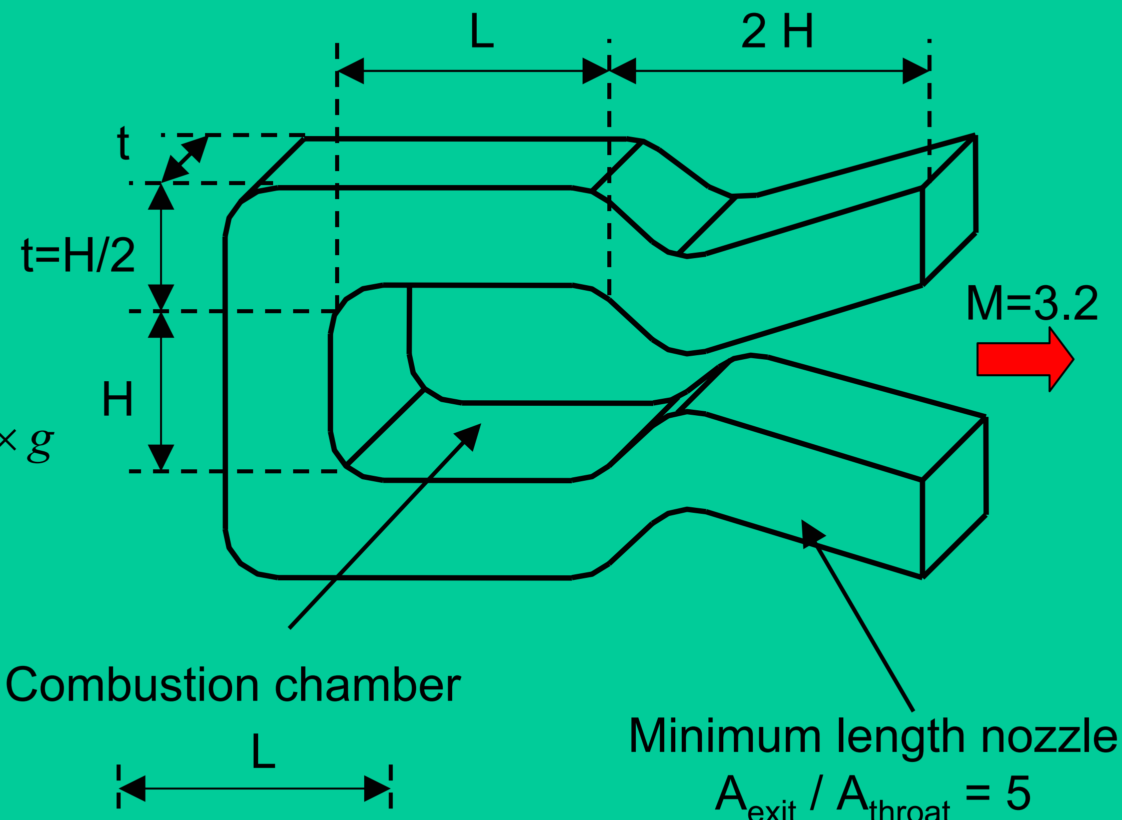
Increasing pressure increases power density

Silicon Micro-Rocket

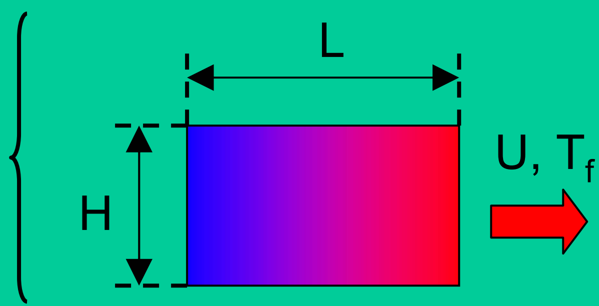
$$T = \dot{m}\left(U_e - U_i\right)$$

$$I_{sp} = U_e / g$$

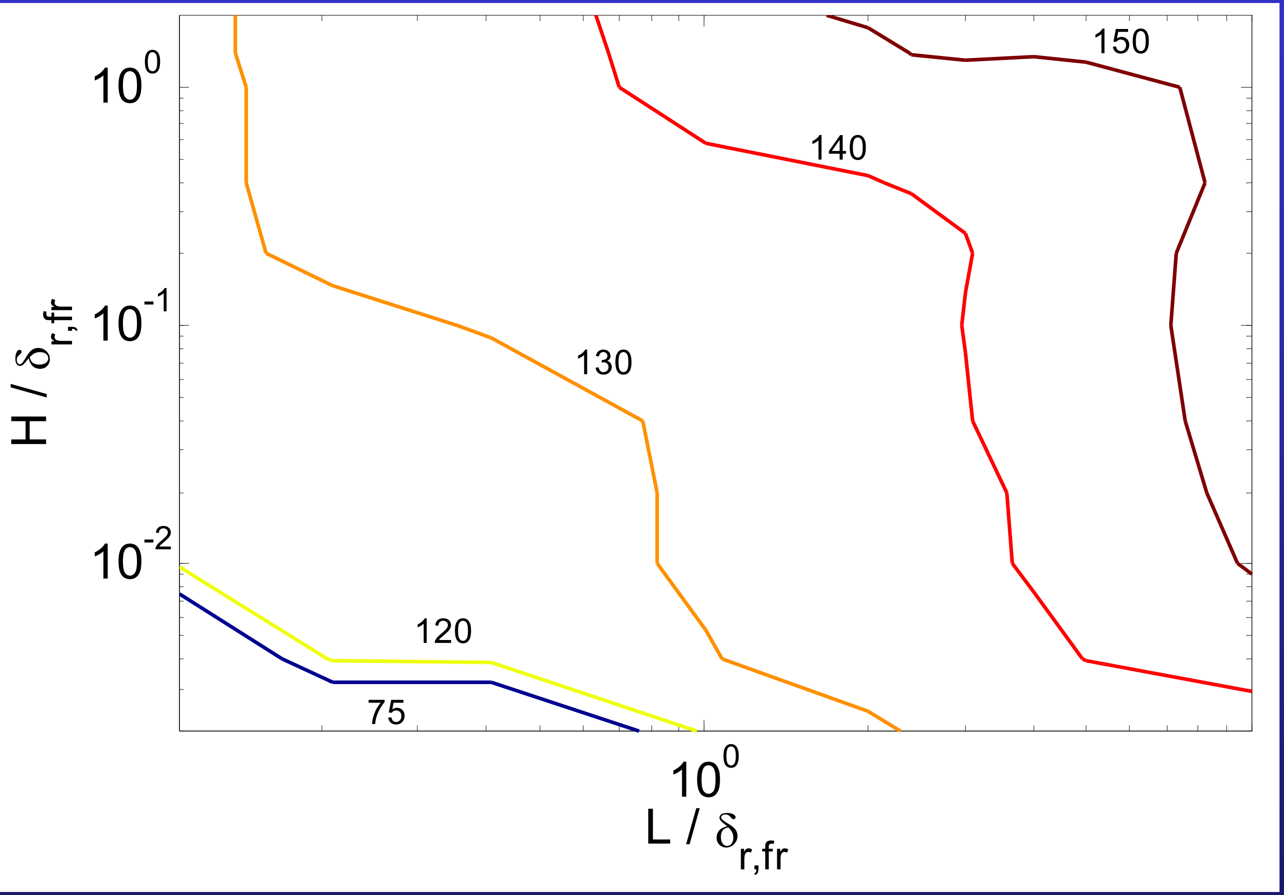
$$Weight = Volume \times \rho_{Si} \times g$$



From numerical computations



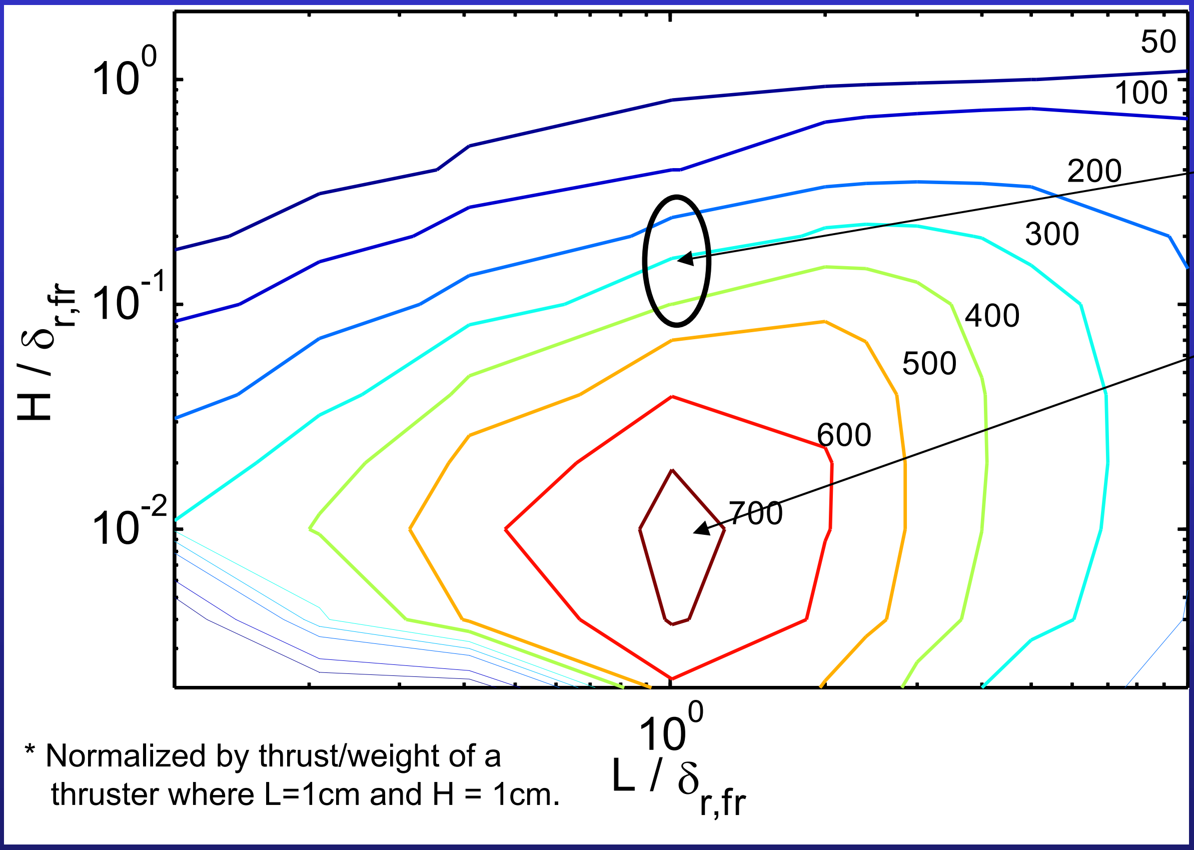
Silicon Micro-Rocket I_{sp}



Maximum I_{sp} at large H and large L

– Reflects trend in combustor efficiency

Silicon Micro-Rocket Thrust/Weight



Practical Design Region?

Optimum Configuration (Neglecting Pressure Loss)

- L=0.5 mm
- H = 5 μm
- T=72x10^{-9} N
- T/W = 943

- *Maximum T/W corresponds to maximum power density*
- *Very high T/W may be possible*

Experiments

- Provide data to validate model and simulations
  - Effect of T_{wall}, $k_{structure}$ on
    - *Burning rate*
    - *Reaction zone thickness*
- Approach
  - Construct parallel plate reactor
    - *Conductive, temperature-controlled walls*
    - *Re-configurable (0.5 mm < H < 10 mm)*
    - *Build using conventional mfg. processes (avoid MEMS)*
  - Develop appropriate diagnostic techniques
    - *Measure temperature and species concentration*
    - *Sub-millimeter spatial resolution*
    - *Non-intrusive*

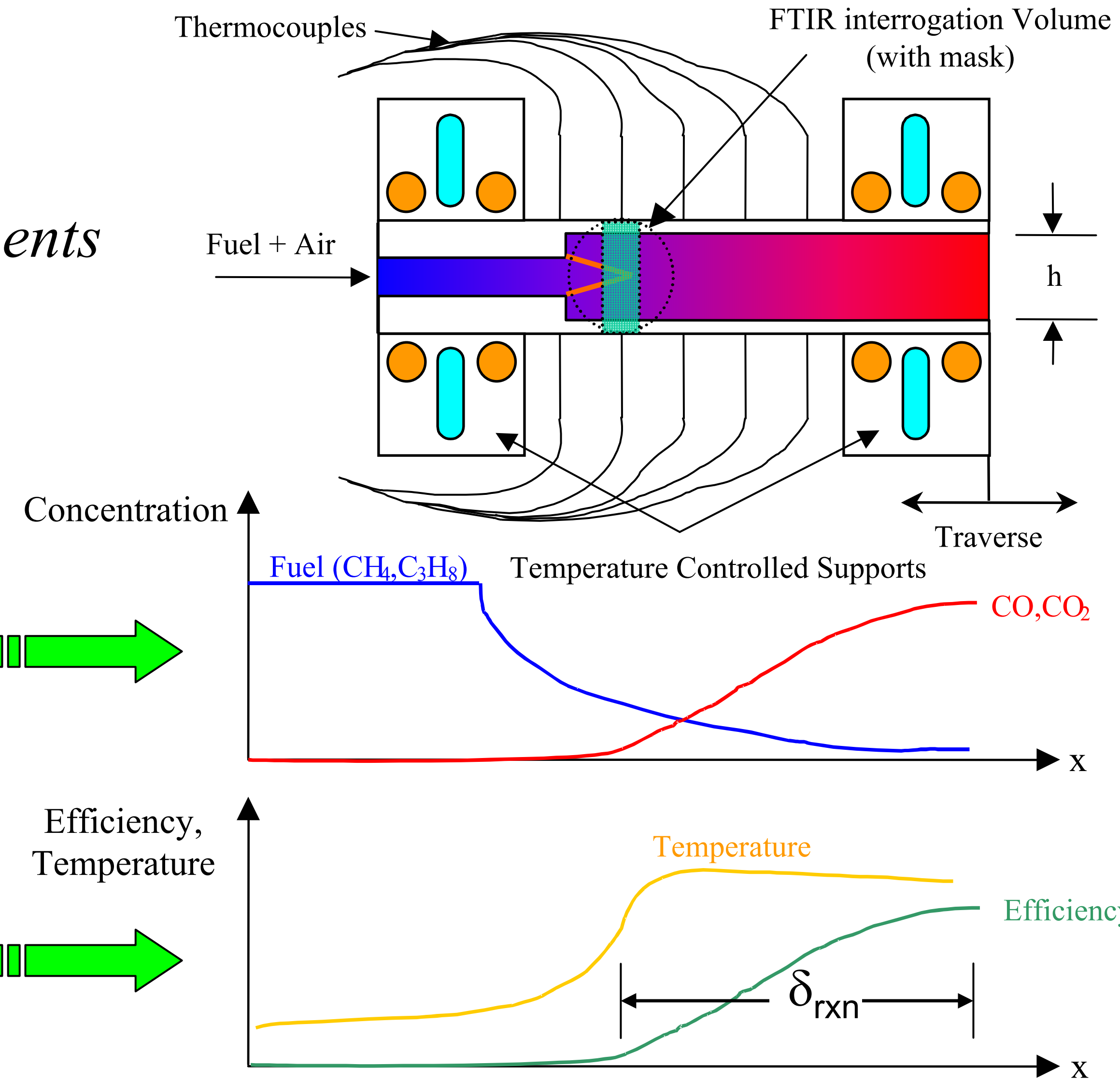
Parallel Plate Reactor

Features:

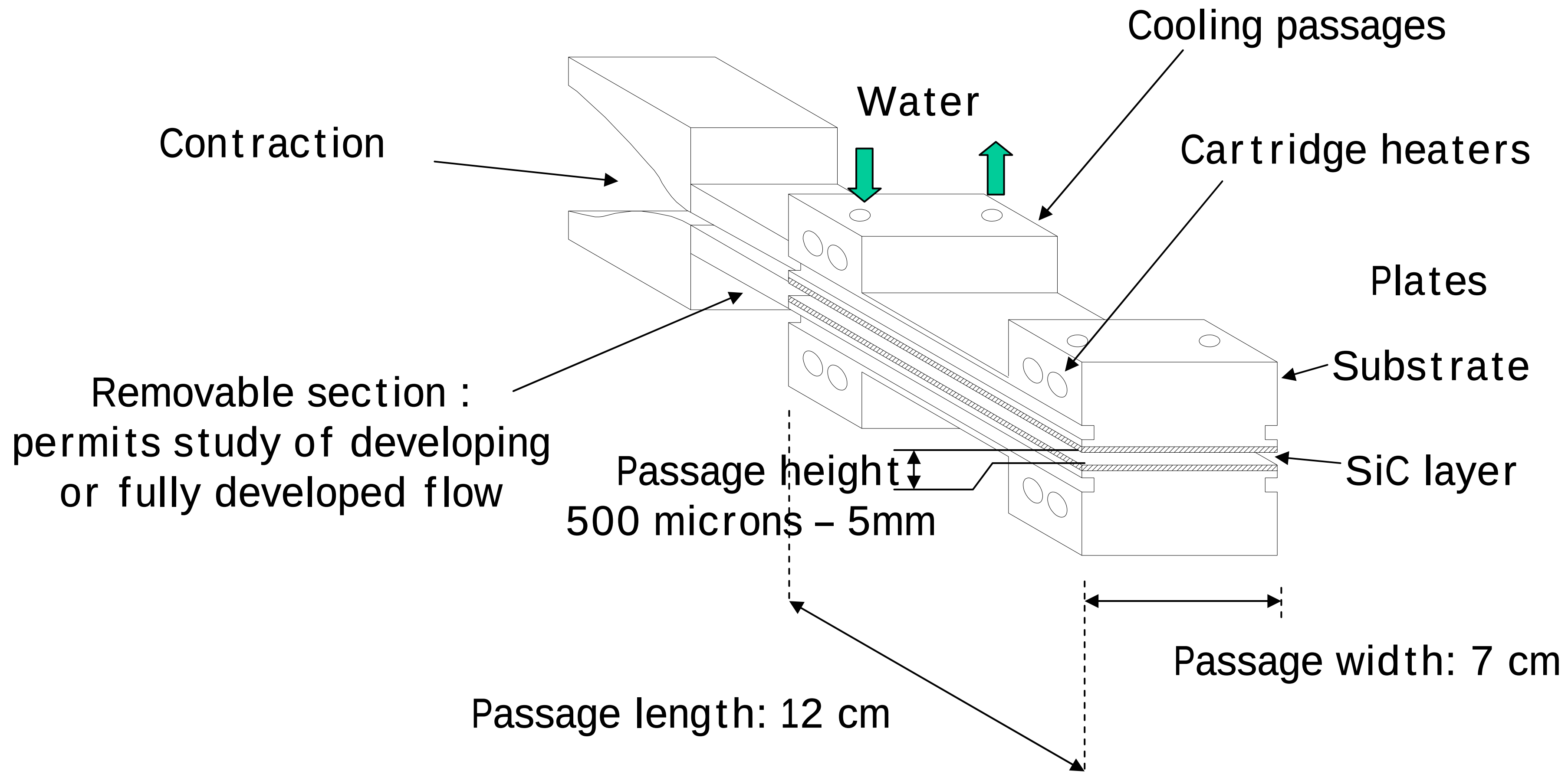
- *Controllable BC's*
- *Detailed Measurements*
    - *Temperature*
    - *Heat Flux*
    - *Species conc.*

Measure

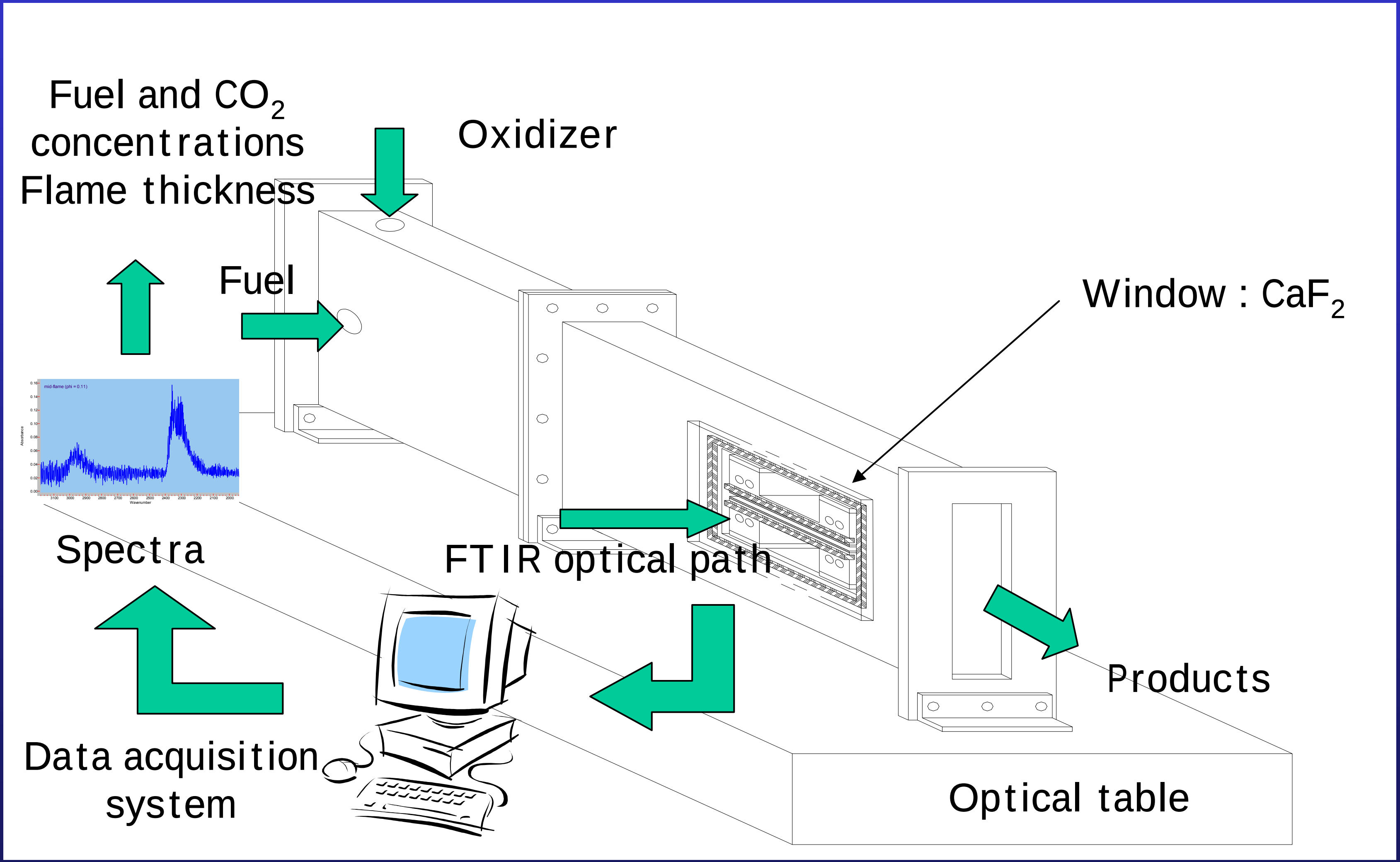
Compute



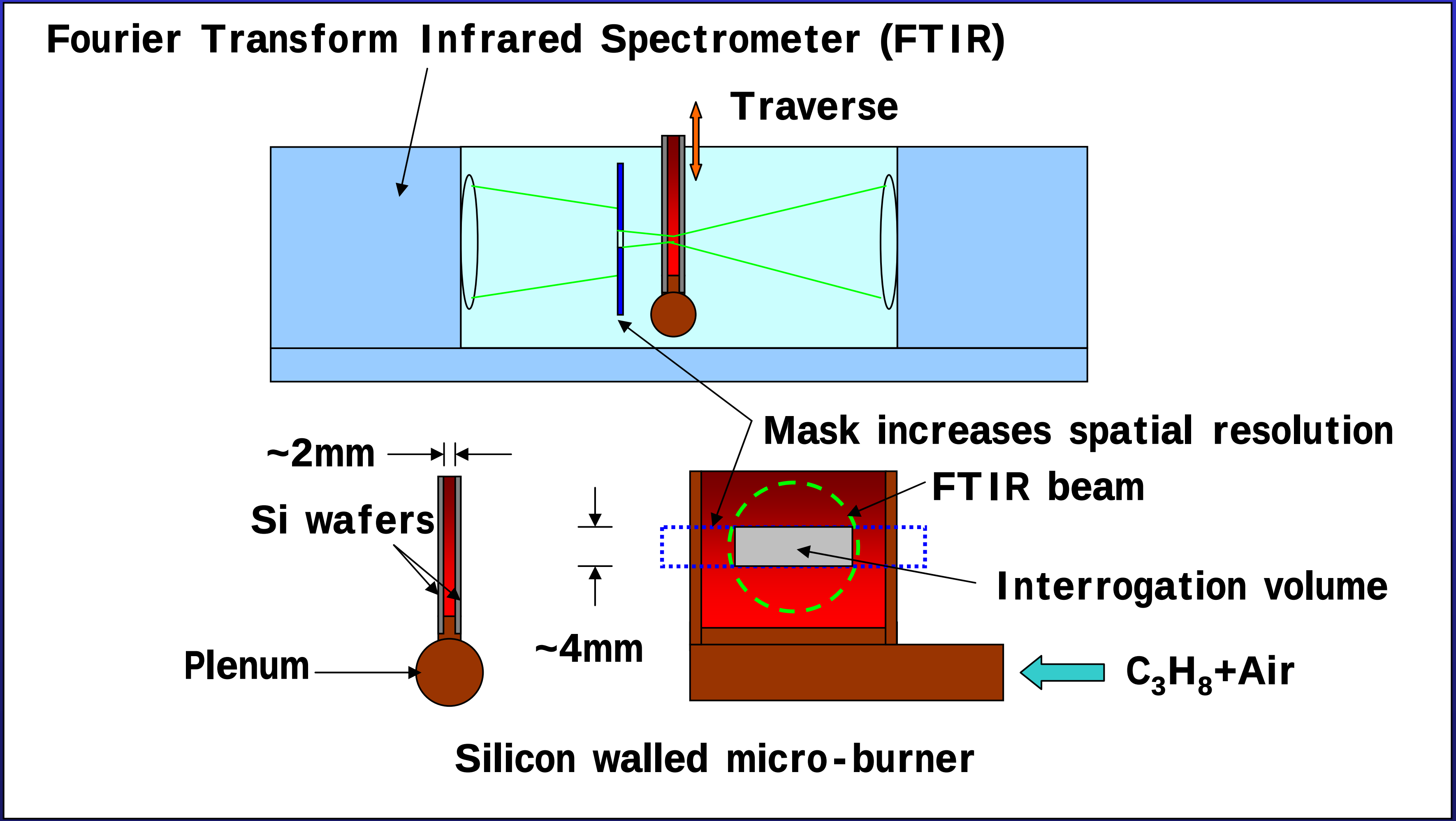
Parallel Plate Reactor



Parallel Plate Reactor



FTIR Proof of Concept



FTIR Proof-of-Concept

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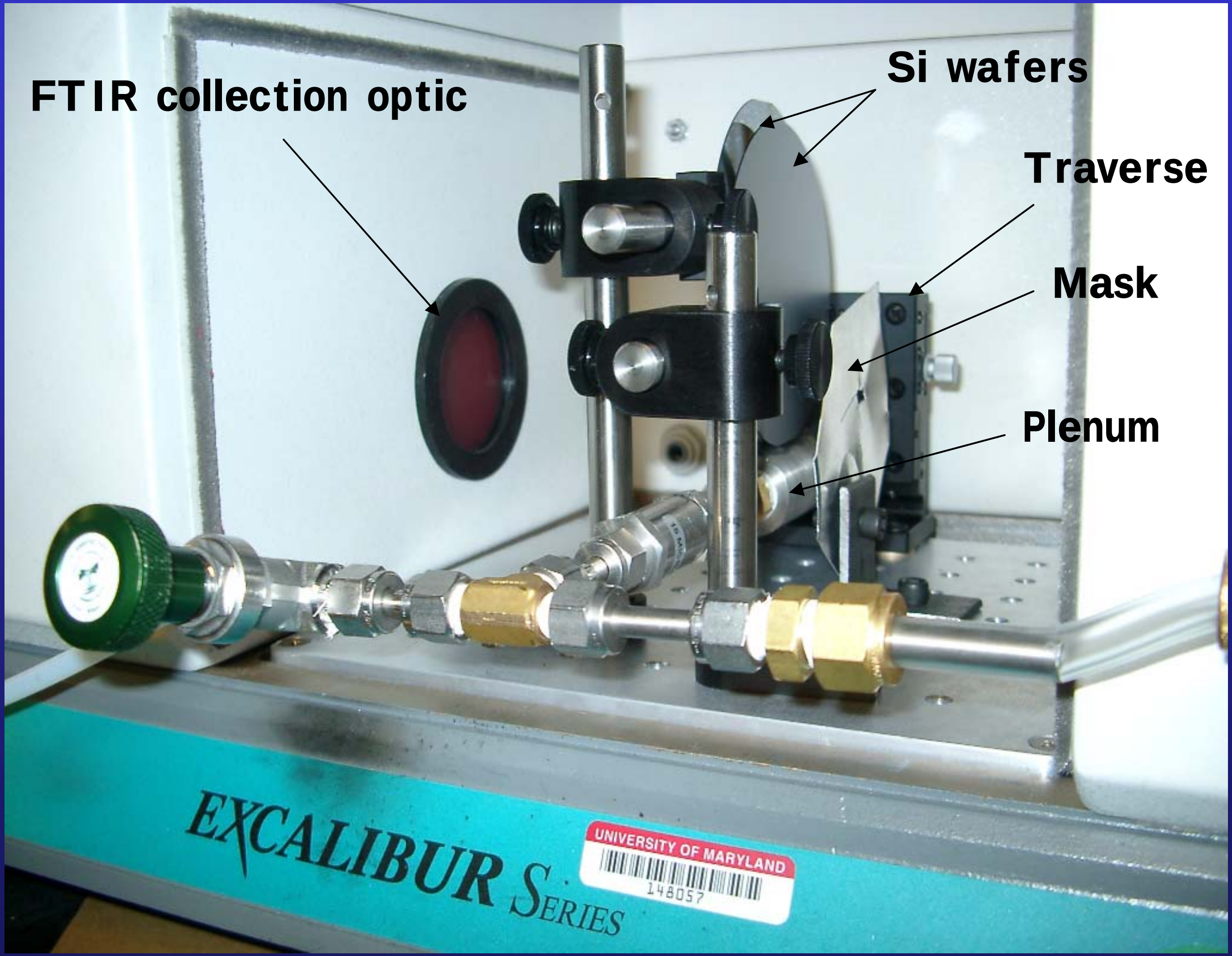
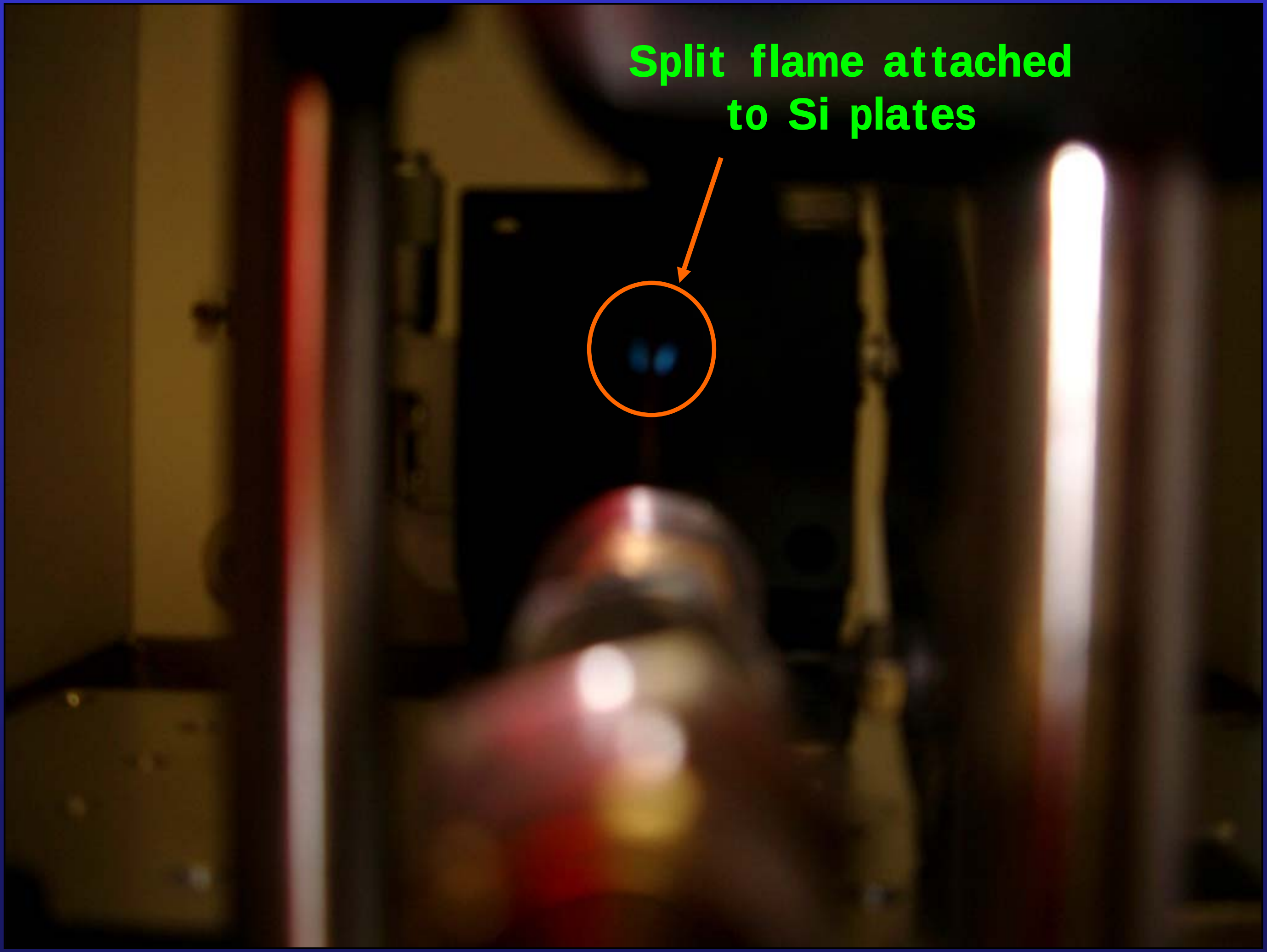
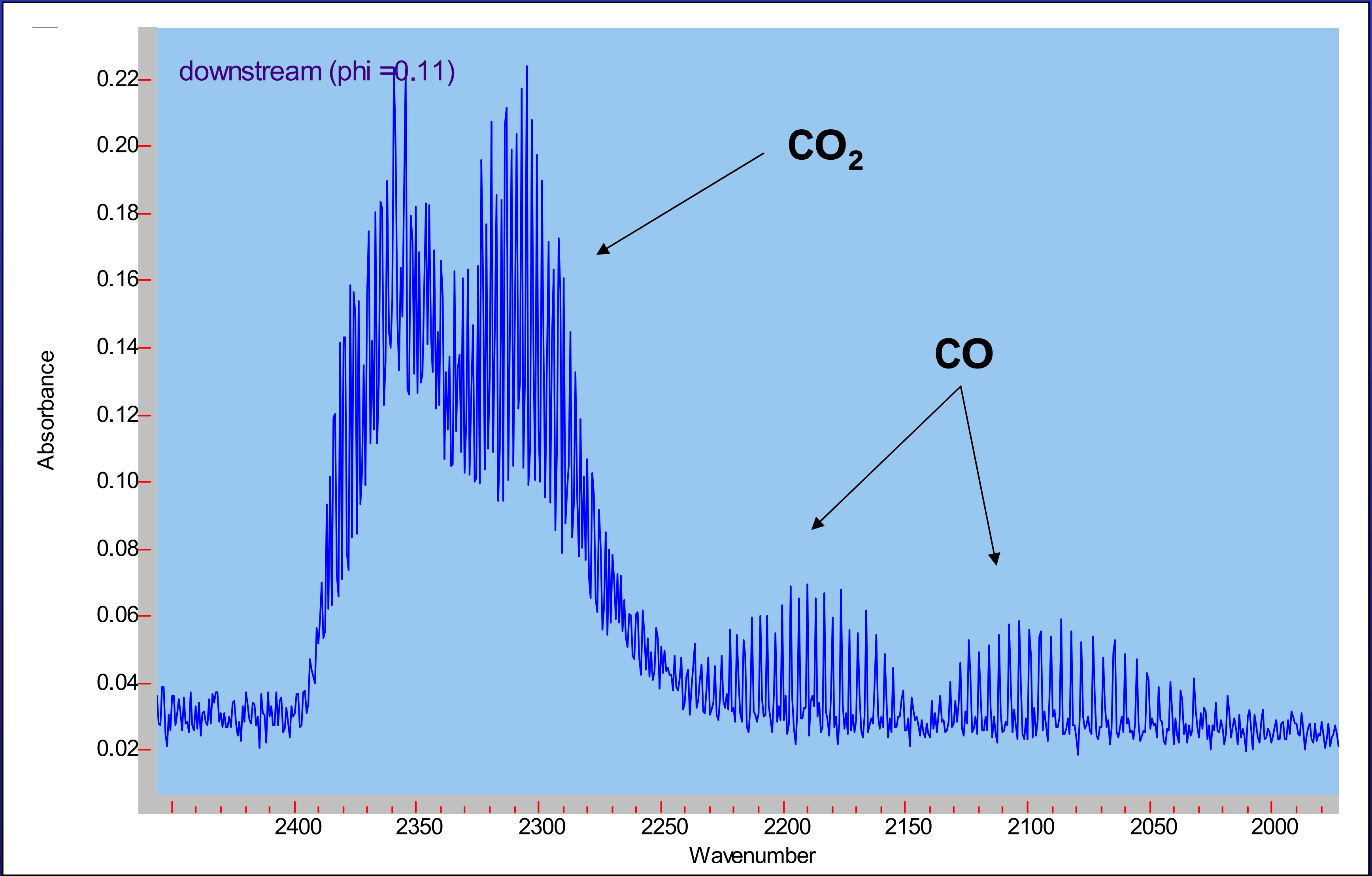


Silicon Micro-burner Operation

U N I V E R S I T Y   O F   M A R Y L A N D



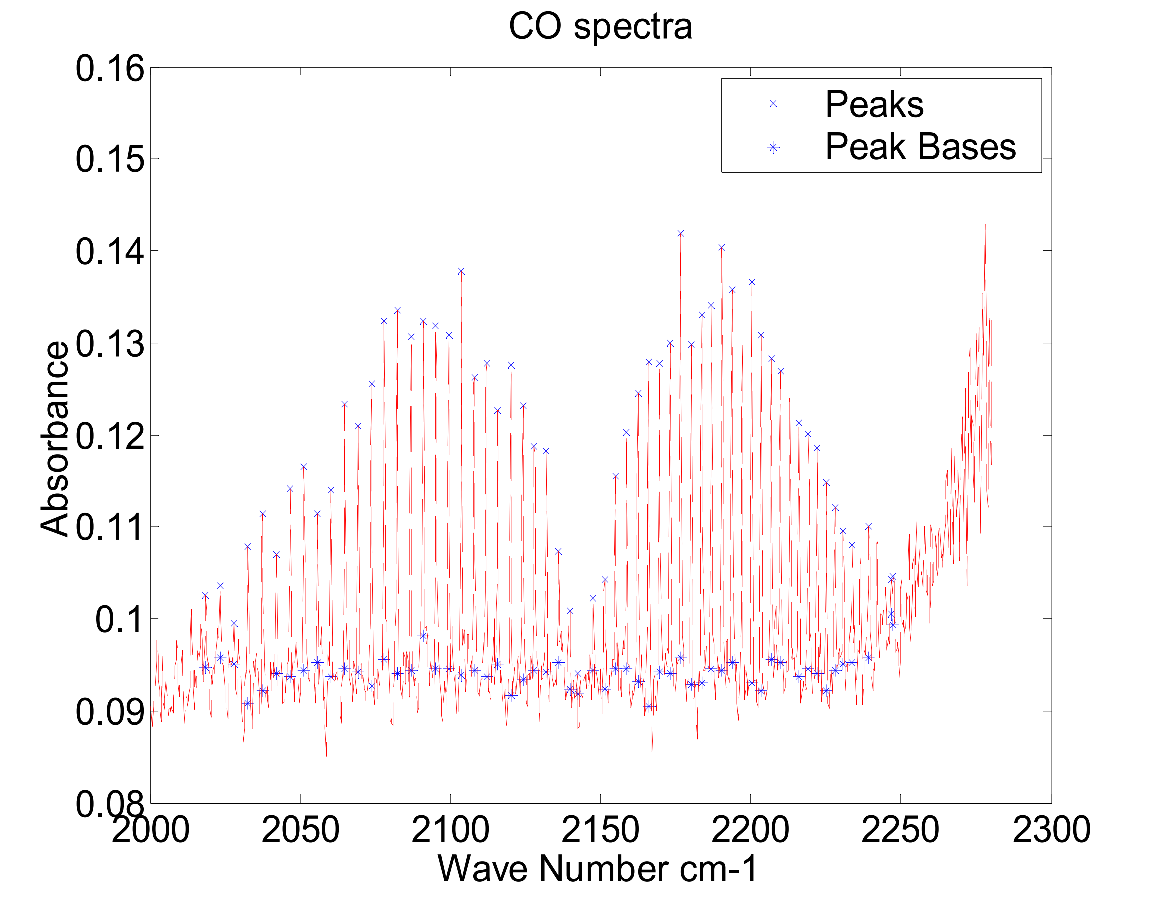
Sample Spectra



Temperature Calculation from CO

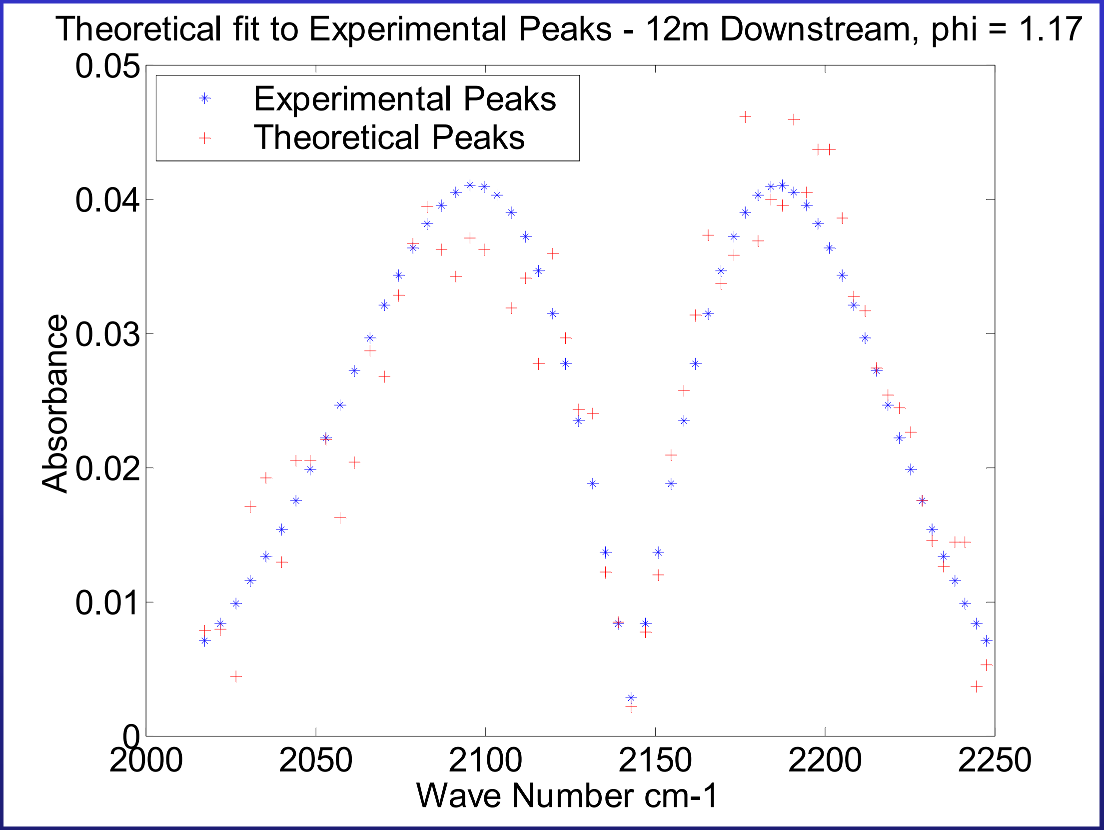
U N I V E R S I T Y O F M A R Y L A N D

1. Identify peaks



Temperature Calculation from CO

2. Fit peaks



$$N_r = (2j+1)\frac{e^{-\frac{E_r(v,j)}{kT}}}{\sum_{j=0}^{\infty}(2j+1)e^{-\frac{E_r(v,j)}{kT}}} \qquad E_r(v,j) = hc\left[B_v j(j+1) - D_v j^2 (j+1)^2\right]$$

Axial Temperature Distribution

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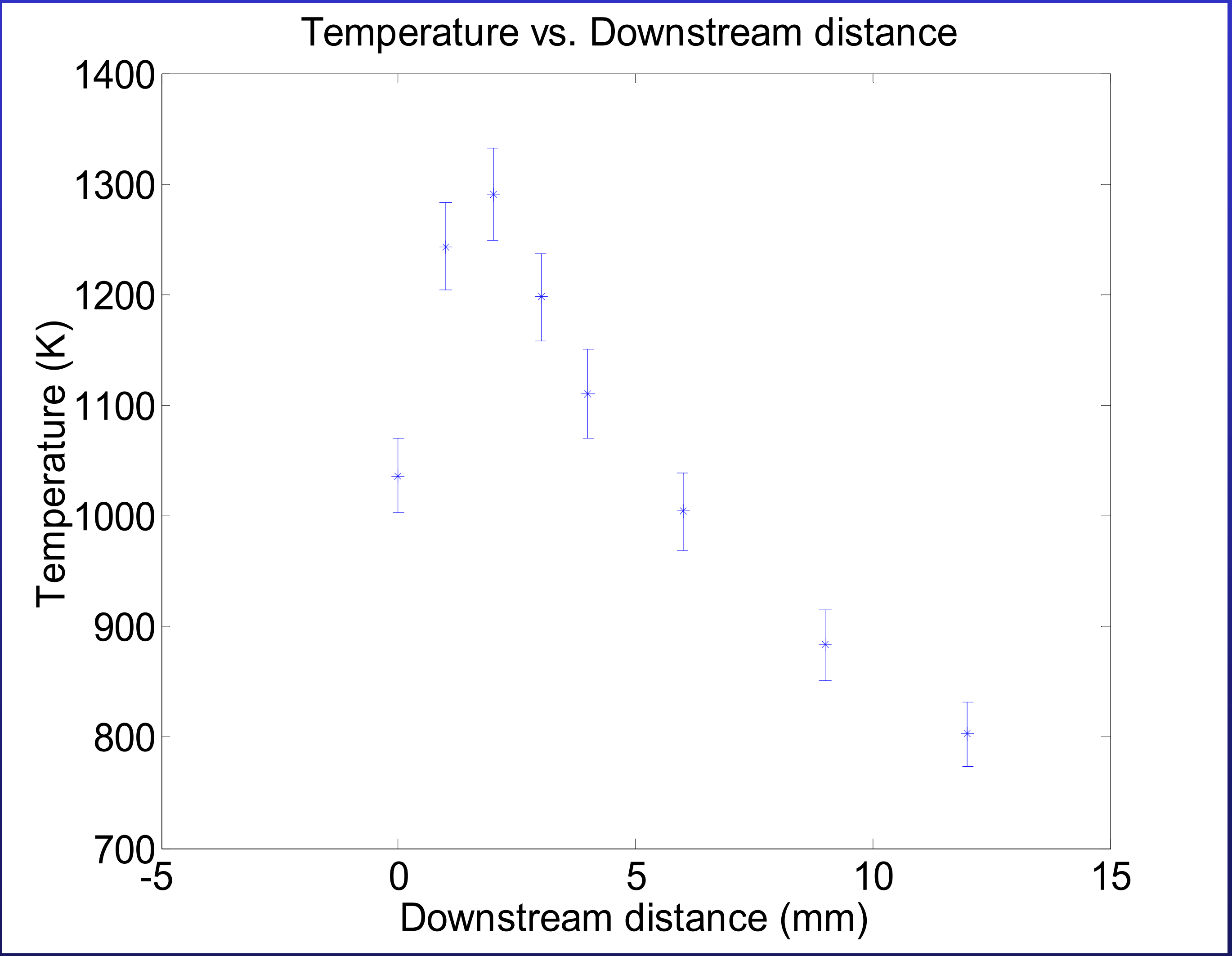

Present Work

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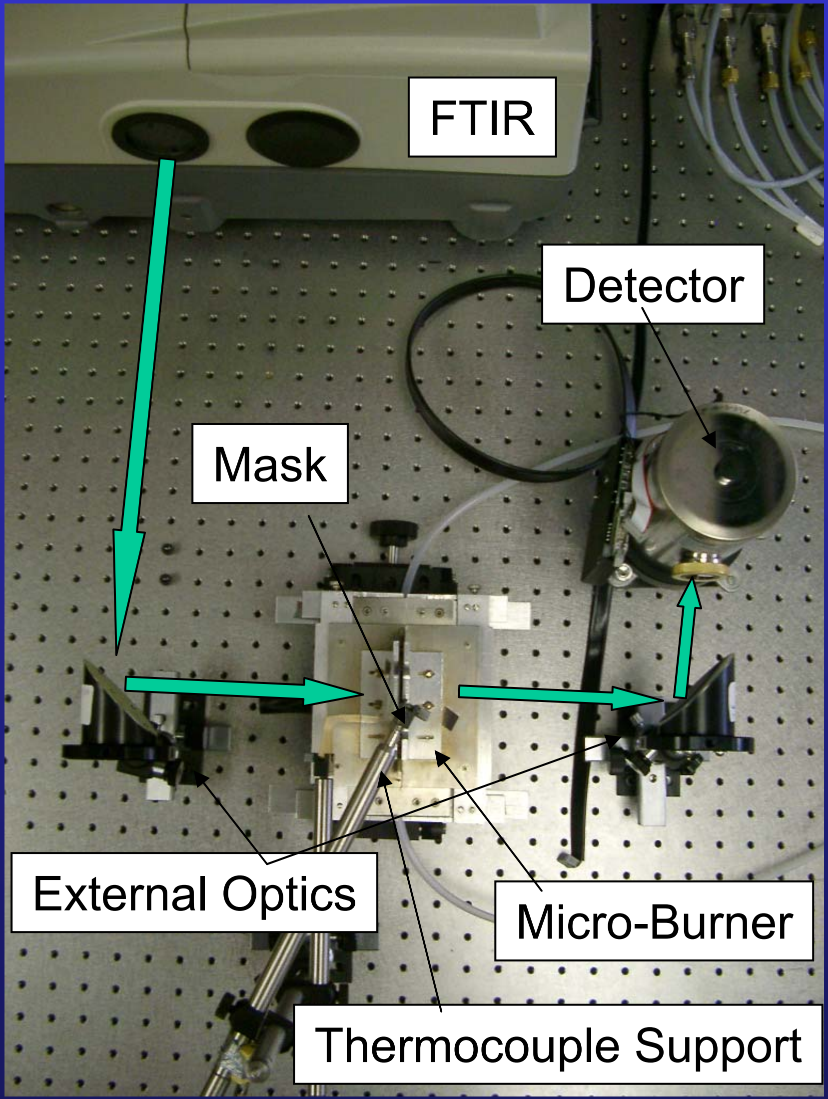
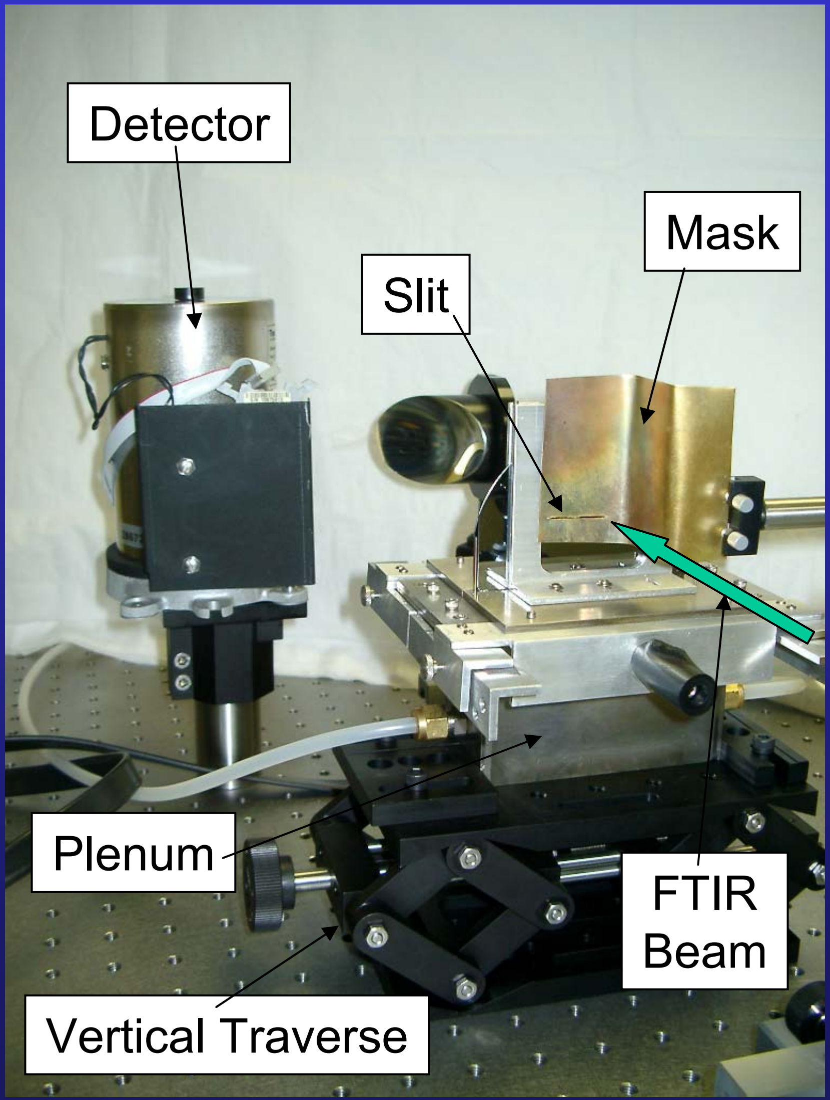


- Improved Optics
  - Better FTIR
  - Higher throughput external beam path
- IR Camera for Plate T
- Improved spectral interpretation

Present Work



- Improved burner
  - Adjustable H
  - Improved traverse
  - Improved flow control

Conclusions

U N I V E R S I T Y O F M A R Y L A N D

- Structural heat conduction has important effects on performance of micro-combustors
  - Increases reaction zone thickness
  - Increases burning rate
  - Leads to optimum power density configurations
    - *Rocket motors with T/W > 400 appear possible*
- Chemical quenching still important
- Viability of micro-rockets hinges on tradeoff between T/W and I_{sp}.
- Experimental verification ongoing

Future Work

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- Simulation
  - Incorporate radiation boundary condition
  - Incorporate surface chemistry
  - Investigate different fuels
- Experiments
  - Measure $\delta_r(H)$ in micro-burner
  - Construct parallel plate flow reactor
  - Replace external optics with optical fiber system

Acknowledgements

The authors would like to thank
Dr. Mitat Birkan and
the Air Force Office of Scientific Research
(AFOSR F496200110435)